Bose-Einstein condensation thermodynamics of a trapped gas with attractive interaction

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We study the Bose-Einstein condensation of an interacting gas with attractive interaction confined in a harmonic trap using a semiclassical two-fluid mean-field model. The condensed state is described by converged numerical solution of the Gross-Pitaevskii equation. By solving the system of coupled equations of this model iteratively we obtain converged results for the temperature dependencies of the condensate fraction, chemical potential, and internal energy for the Bose-Einstein condensate of ^{7}Li atoms.

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I. INTRODUCTION

There has been recent experimental observation of Bose-Einstein (BE) condensation in dilute interacting bosonic atoms of ^{87}Rb [1,2], ^{23}Na [3], ^{7}Li [4,5], and ^{1}H [6] employing magnetic traps at ultra-low temperatures. The interaction among the atoms could be either attractive or repulsive. Although, in both cases the condensate is well-described by the Gross-Pitaevskii (GP) equation [7,8], the nature of BE condensates in these two cases is of entirely different nature. In the repulsive case the number of atoms in the condensate can grow without bound, whereas this number is limited by a upper bound in the case of attractive interaction [9–11]. Of the experimentally observed cases of BE condensation one has repulsion for ^{1}H, ^{23}Na, and ^{87}Rb atoms and attraction for ^{7}Li atoms. The existence of a maximum number of condensed atoms in the case of ^{7}Li has been noted experimentally and is consistent with the prediction of theoretical analysis based on the GP equation [5,9–13]. In the attractive case the GP equation has no solution for the number of atoms larger than a critical number.

The GP equation is a nonlinear Schrödinger equation and it is tedious to find its converged numerical solution [12–17]. For the repulsive case, an approximate solution scheme of this equation, such as the one based on the Thomas-Fermi approximation, has frequently been used for a qualitative description of the condensate [18]. However, no such approximation scheme is known for the attractive case which requires an exact numerical solution of the GP equation. This makes the theoretical study of this case a more challenging task.

There have been several comprehensive studies on the temperature dependencies of the thermodynamic observables in the case of repulsive interaction using mean-field two-fluid models [18–21]. One such mean-field scheme is provided by the so-called Popov approximation [22] and has been considered by several authors [19–21,23,24]. The physical ingredients of these mean-field models [18–21,23,24] are quite similar and they lead to similar numerical results in the case of weakly repulsive interatomic interactions.

We shall use a two-fluid mean-field model [18] to study the temperature dependencies of the thermodynamic observables of the condensate. For a condensate composed of 40000 trapped ^{87}Rb atoms the perturbative solution of the system of equations of this model converged rapidly and provided a satisfactory account of the condensate fraction, internal energy, and specific heat in agreement with experiment [1,2]. It was also found that the lowest order solution already provided a very good approximation. Later the same model has been used in one and two space dimensions [25,26].

The above mean-field two-fluid model [18] is used in this work for a theoretical description of the BE condensation thermodynamics in the case of attractive interaction appropriate for ^{7}Li. Depending on the strength of the attractive potential, the condensate in the attractive case may consist of a few thousand atoms confined by the trap potential. For a fixed trap, the maximum number of atoms in the BE condensate with attractive interaction is inversely proportional to $|a|$ [23], where a is the scattering length of two atoms. As the temperature is lowered below the critical temperature T_0 of BE condensation, the condensate starts to form and finally at 0 K all the available atoms (limited by the maximum number mentioned above) form the condensate in the present model.

The condensate wave function in the present model is described by the GP equation. In the repulsive case usually some approximate solutions of the GP equation are used [18,19,23]. Although we shall be using the iterative solution of the system of equations of the mean-field model, we shall employ a converged numerical solution of the GP equation in the present attractive case. As the GP equation is a nonlinear one, this amounts to a nontrivial modification of the calculational scheme.

The plan of the paper is as follows. In Sec. II we present the mean-field two-fluid model. In Sec. III we discuss the numerical scheme for its solution and present numerical results for ^{7}Li. Finally, in Sec. IV we present some concluding remarks.

II. MEAN-FIELD TWO-FLUID MODEL

We consider a system of N bosons with attractive interaction at temperature T under the influence of a trap potential. The condensate is described by the following GP equation for the wave function $\Psi(\mathbf{r})$ with eigenvalue $\bar{\mu}$ [7,8,18,23]:

$$\left[-\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(r) + 2gn_1(r) + g\Psi^2(\mathbf{r}) - \bar{\mu} \right] \Psi(\mathbf{r}) = 0. \tag{2.1}$$

Here $V_{\text{ext}}(r) \equiv m\omega^2 r^2/2$ is the spherically symmetric harmonic-oscillator trap potential, $g \equiv 4\pi\hbar^2 a/m$ the strength of the interatomic interaction, m the mass of a single atom, ω the angular frequency, a the atom-atom scattering length, $\mu \equiv \bar{\mu} - \bar{\mu}_0$ is the chemical potential, where $\bar{\mu}_0$ is the eigenvalue of Eq. (2.1) for the harmonic oscillator potential alone in the absence of interatomic interaction ($g = 0$), and $n_1(r)$ represents the distribution function of the noncondensed bosons. Although in actual experiment [5] the harmonic oscillator trap is not quite symmetric, the deviation from spherical symmetry is quite small. However, the converged numerical solution of the GP equation (2.1) for a nonsymmetric trap is quite complicated numerically and hence for a qualitative description we consider a spherically symmetric trap in the present study. An attractive (repulsive) interaction corresponds to negative (positive) values of a and g.

The noncondensed particles are treated as noninteracting bosons in an effective potential $V_{\text{eff}}(r) = V_{\text{ext}}(r) + 2gn_1(r) + 2g\Psi^2(\mathbf{r})$ [27]. Thermal averages are calculated with a standard Bose distribution of the noncondensed particles in chemical equilibrium with the condensate governed by the same chemical potential μ. In particular the density $n_1(r)$ is given by [27]

$$n_1(r) = \frac{1}{(2\pi\hbar)^3} \int \frac{d^3p}{\exp[\{p^2/2m + V_{\text{eff}}(r) - \mu\}/k_B T] - 1}, \tag{2.2}$$

where k_B is the Boltzmann constant. Equations (2.1) − (2.2) above are the principal equations of the present model.

The total number of particles N of the system is given by

$$N = N_0 + \int \frac{\rho(E)dE}{\exp[(E - \mu)/k_B T] - 1}, \tag{2.3}$$

where $N_0 \equiv \int \Psi^2(\mathbf{r})d^3r$ is the total number of particles in the condensate. The semiclassical density of states $\rho(E)$ of Eq. (2.3) is given by [27]

$$\rho(E) = \frac{(2m)^{3/2}}{4\pi^2\hbar^3} \int_{V_{\text{eff}}(r) < E} \sqrt{E - V_{\text{eff}}(r)}d^3r. \tag{2.4}$$

The critical temperature T_0 is obtained as the solution of Eq. (2.3) with N_0 and μ set equal to 0.

The average single-particle energy of the noncondensed particles is given by [18]

$$\langle E \rangle_{\text{nc}} = \int \frac{E\rho(E)dE}{\exp[(E - \mu)/k_B T] - 1}. \tag{2.5}$$

The kinetic energy of the condensate is assumed to be negligible and its interaction energy per particle is given by $\langle E \rangle_{\text{c}} = (g/2) \int \Psi^4(\mathbf{r})d^3r$. The quantity of experimental interest is the average total energy $\langle E \rangle = [\langle E \rangle_{\text{nc}}(N - N_0)/2 + \langle E \rangle_{\text{c}}]/N$, which we calculate.

The coupling of the nonlinear equation (2.1) with other equations make the solution algorithm complicated and it is convenient to express this system of equation in dimensionless units. This has advantage in the numerical solution [16,17]. We express energy in units of $\hbar\omega$, and length in units of the harmonic oscillator length $a_{\text{ho}} \equiv \sqrt{\hbar/(m\omega)}$. We shall consider in this paper only the spherically symmetric ground state solution of the condensate with $\Psi(\mathbf{r}) = \Psi(r)$. Then the GP equation (2.1) become

$$\left[-\frac{d^2}{dx^2} + x^2 + 4\pi\eta\bar{n}_1(x) \pm \frac{2\phi^2(x)}{x^2} - 2\bar{\alpha} \right] \phi(x) = 0, \tag{2.6}$$

where $\eta \equiv 4a/a_{\text{ho}}$ is the new dimensionless strength, $x \equiv r/a_{\text{ho}}$, $\Psi(r) \equiv \phi(x)/(x\sqrt{\pi|\eta|a_{\text{ho}}^3})$, and $\bar{\alpha} \equiv \bar{\mu}/(\hbar\omega)$. The positive (negative) sign in Eq. (2.6) corresponds to repulsive (attractive) interaction. The dimensionless density $\bar{n}_1(x) \equiv a_{\text{ho}}^3 n_1(r)$ is defined by

$$\bar{n}_1(x) = \frac{1}{2\pi^2} \int \frac{k^2 dk}{\exp[\{k^2/2 + V_{\text{eff}}(x) - \alpha\}/t] - 1}, \tag{2.7}$$

where $k \equiv pa_{\text{ho}}/\hbar$, $V_{\text{eff}}(x) \equiv x^2/2 + 2\pi\eta\bar{n}_1(x) + 2\phi^2(x)/x^2$, $t \equiv k_B T/(\hbar\omega)$, $\alpha \equiv \mu/(\hbar\omega)$. For the spherically symmetric ground state $\alpha = \bar{\alpha} - \bar{\alpha}_0$, where $\bar{\alpha}_0 \equiv \bar{\mu}_0/(\hbar\omega) = 1.5$ is the energy eigenvalue of the harmonic oscillator potential alone (zero-point energy in units of $\hbar\omega$) in the absence of interatomic interaction. In the present consideration of the chemical potential finite-size effects are excluded [18,19]. Using these dimensionless variables the number equation (2.3) becomes

$$N = N_0 + \int \frac{\bar{\rho}(e)de}{\exp[(e - \alpha)/t] - 1}, \tag{2.8}$$

where $N_0 = (4/|\eta|) \int \phi^2(x)dx$, $e \equiv E/(\hbar\omega)$, and the dimensionless density $\bar{\rho}(e) \equiv \hbar\omega\rho(E)$ is given by

$$\bar{\rho}(e) = \frac{2\sqrt{2}}{\pi} \int_{V_{\text{eff}}(x) < e} \sqrt{e - V_{\text{eff}}(x)}x^2 dx. \tag{2.9}$$

The above set of equations (2.6) − (2.9) are solved iteratively using the converged numerical solution of the GP

equation (2.6). The iteration is started with $\bar{n}_1(x) = 0$ at a definite temperature with a trial value for the chemical potential α. Then Eq. (2.6) is solved and with its solution the functions $V_{\text{eff}}(x)$ and $\bar{n}_1(x)$ are calculated. Using these new $V_{\text{eff}}(x)$ and $\bar{n}_1(x)$ Eq. (2.6) is solved again and $\bar{n}_1(x)$ and $\phi(x)$ are recalculated. This iterative scheme is continued until final convergence is achieved. In each order of iteration we calculate the condensate fraction N_0/N and energy $\langle E \rangle$, in addition to the chemical potential α. This scheme is repeated until convergence is achieved. It is then verified if the number equation (2.8) is satisfied with this solution. If not, a new trial value for the chemical potential is employed. Once the number equation is satisfied the desired solution is obtained.

Next we present the solution procedure of the GP equation (2.6). The solution of this equation satisfies the following boundary conditions [14,15]

$$\phi(0) = 0, \qquad \phi'(0) = \text{constant} \qquad (2.10)$$

$$\lim_{x \to \infty} \phi(x) = N_C \exp\left[-\frac{x^2}{2} + \left(\bar{\alpha} - \frac{1}{2}\right)\ln x\right], \qquad (2.11)$$

where N_C is a normalization constant. The derivative of the wave function can be obtained from Eq. (2.11) and one obtains the following log-derivative of the wave function in the asymptotic region

$$\lim_{x \to \infty} \frac{\phi'(x)}{\phi(x)} = \left[-x + \left(\bar{\alpha} - \frac{1}{2}\right)\frac{1}{x}\right]. \qquad (2.12)$$

Equation (2.6) is integrated numerically for a given $\bar{\alpha}$ by the four-point Runge-Kutta rule starting at the origin ($x = 0$) with the initial boundary condition (2.10) with a trial $\phi'(0)$ in steps of $dx = 0.001$. Using Eq. (2.6) the integration is propagated to $x = x_{\text{max}}$, where the asymptotic condition (2.12) is valid. The agreement between the numerically calculated log-derivative of the wave function and the theoretical result (2.12) is enforced to four significant figures. The maximum value of x up to which we need to integrate to obtain this precision is $x_{\text{max}} = 3$. If for a trial $\phi'(0)$, this precision can not be obtained, a new value of $\phi'(0)$ is to be chosen. The procedure is repeated until the converged solution is obtained.

III. NUMERICAL RESULTS

In our numerical study we would be interested only in the case of attractive interaction (negative η). We consider the experimentally relevant situation of ^{7}Li [4,5]. In this case the trap frequencies in the experiment of Ref. [5] along the X, Y, and Z directions are 150.6 Hz, 152.6 Hz, and 131.5 Hz which lead to a maximum of about 1400 trapped atoms. The deviation from spherical symmetry in this case is small and in order to have a qualitative understanding of the condensate we consider the trap to be spherically symmetric with $N_{\text{max}} = 1400$. We

reconfirm from the numerical solution of the GP equation that [23]

$$\frac{|\eta|N_{\text{max}}}{4} = 0.575. \qquad (3.1)$$

Considering the known result for ^{7}Li, that $N_{\text{max}} = 1400$ [5], we obtain from Eq. (3.1), $\eta = -0.00164$ and we use this value of η in our numerical calculation. In our calculation we use three values of N, e.g., $N = 1300, 1000$, and 500 ($N < N_{\text{max}} = 1400$). First we calculate the critical temperatures in these cases from the number equation (2.8) and obtain the values $T_0 = 10.27\hbar\omega/k_B, 9.41\hbar\omega/k_B, 7.47\hbar\omega/k_B$ for $N = 1300, 1000$ and 500, respectively.

In the case of ^{7}Li, the estimated value of $\eta(= -0.00164)$ is quite small. This corresponds to a very weak coupling and we find that the lowest-order solution is graphically almost indistinguishable from the converged solution for the condensate fraction, chemical potential, and total energy. The estimated coupling η for ^{87}Rb is 0.0248 [1,2,18], which is more than ten times larger in magnitude than the coupling for ^{7}Li. In the case of ^{87}Rb, already the lowest order result was very good [18,23]. Hence the very rapid convergence of the present results is not quite unexpected. In the present study we only exhibit the converged result after two iterations.
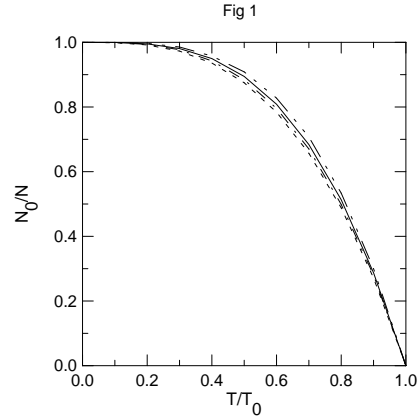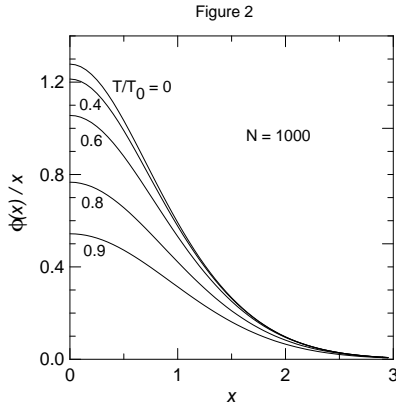

Fig. 1. Converged condensate fraction N_0/N as a function of T/T_0 for $\eta = -0.00164$ and $N = 1300$ (full line) and 500 (dashed-dotted line); for $\eta = -0.01$ and $N = 200$ (dashed-double-dotted line); and for trapped ideal Bose gas (dotted line).

In Fig. 1 we present the temperature (T/T_0) dependence of the condensate fraction N_0/N for ^{7}Li with $\eta = -0.00164$ for $N = 1300$ and 500. The result for $N = 1000$ is indistinguishable from that of $N = 1300$. The result for $\eta = 0$ corresponding to an ideal Bose gas in a harmonic trap is also shown in this figure. For comparison, the result in the case of a stronger attractive interaction for $\eta = -0.01$ and $N = 200$ is also shown. In the case of repulsive interaction, the result for N/N_0 at a particular temperature T/T_0 is smaller than that for an ideal Bose gas [23]. In the present case of attractive interaction, the result for N/N_0 at a particular tempera-

ture T/T_0 is larger than that for the ideal Bose gas. We also find from this figure that, as expected, the result for the stronger attractive interaction ($\eta = -0.01$) deviates more from the ideal gas result than in the case of ^{7}Li ($\eta = -0.00164$). We did not consider a much stronger attractive coupling, as because of Eq. (3.1) this would correspond to an unacceptably small value for the number of particles in the condensate. This number is already small for the case $\eta = -0.01$ considered in this work.

As the solution of the GP equation (2.6) in this case is nontrivial, we show in Fig. 2 the wave functions $\phi(x)/x$ for $N = 1000$ at temperatures $T/T_0 = 0$, 0.4, 0.6, 0.8, and 0.9. As temperature decreases, the wave function is more pronounced corresponding to an increase in the number of particles N_0 in the condensate given by the normalization $N_0 = (4/|\eta|) \int \phi^2(x) dx$. For other values of N, the wave functions are similar to those in Fig. 2 and we do not show these wave functions here.


Fig. 2. GP wave function $\phi(x)/x$ of Eq. (2.6) for $N = 1000$ at different temperatures T/T_0 for $\eta = -0.00164$.
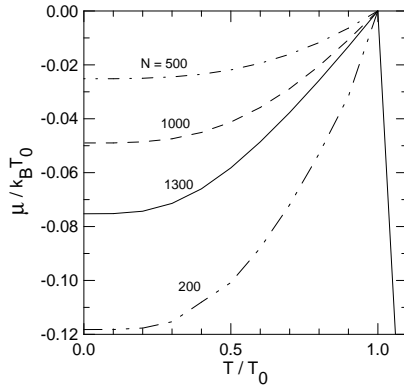
Fig. 3. Chemical potential $\mu/(k_B T_0)$ as a function of T/T_0 for $\eta = -0.00164$ and $N = 1300$ (full line), 1000 (dashed line) and 500 (dashed-dotted line); and for $\eta = -0.01$ and $N = 200$ (dashed-double-dotted line).

In Fig. 3 we show the chemical potential of the system at different temperatures T/T_0 for $N = 1300, 1000$, and 500 and $\eta = -0.00164$. For comparison we also show the result for the stronger attractive interaction with $N = 200$ and $\eta = -0.01$. Above the critical tem-

perature $T > T_0$, the chemical potential for a trapped ideal Bose gas is negative and it becomes zero at the critical temperature [23]. The same is true in the present simplified model where the very weakly interacting non-condensed gas is taken to be noninteracting. The only effect of interaction is considered via the condensate. The effect of the interaction among the atoms of the noncondensed gas could be important for T just below T_0 when there will be a large fraction of noncondensed gas and a small fraction of condensed gas. For T close to 0 when most atoms are condensed such effect could be neglected. At present a correct description of BEC thermodynamics including the interaction among noncondensed atoms is beyond the scope of the present work. Hence, although it would be more appropriate to treat the noncondensed gas to be interacting, the effect of interaction in the treatment of the noncondensed gas is expected to be negligibly small in the present study of very weakly interacting Bose gas ($\eta = -0.0164$) and is neglected. In the case of the ideal Bose gas, below the critical temperature the chemical potential is identically equal to zero. For the present case of the trapped Bose gas with attractive interaction, the chemical potential, after becoming zero at $T = T_0$ from a negative value, becomes negative again as the temperature is reduced below the critical temperature. The chemical potential for the stronger attractive interaction ($\eta = -0.01$) deviates more from the trapped ideal gas result ($\mu = 0$) below the critical temperature, than in the case of the weak attractive interaction of ^{7}Li ($\eta = -0.00164$). In the case of repulsive interaction, the chemical potential becomes positive for temperatures below $T = T_0$ [23].
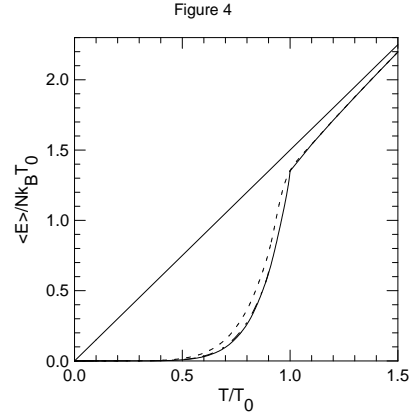
Fig. 4. Energy $\langle E \rangle/(Nk_B T_0)$ as a function of T/T_0 for $\eta = -0.00164$ and $N = 1300$ (full line) and 500 (dashed-dotted line); for $\eta = 0.00164$ and $N = 1300$ (dotted line); and the classical Maxwell-Boltzmann distribution (straight line).

In Fig. 4 we plot the temperature dependence of energy $\langle E \rangle/(Nk_B T)$ for $\eta = -0.00164$ and $N = 1300$ and 500. These two cases lead to almost identical energies as can be seen from Fig. 4. For comparison, in this figure we also show the result for the repulsive interaction for $\eta = 0.00164$ and $N = 1300$. The energy for

the trapped ideal Bose gas should lie between the energies for the attractive and repulsive cases mentioned above. The classical Maxwell-Boltzmann result is also shown. For Bose-Einstein condensation to materialize the energy of the system should be lower that the classical result. The energy in the attractive case is smaller than the corresponding repulsive case below critical temperature [18,23].

IV. CONCLUSION

In conclusion, we studied the temperature dependence of condensate fraction, chemical potential, and total energy for a trapped ^{7}Li gas consisting of 1300, 1000, and 500 atoms with attractive interaction using a mean-field two-fluid model. The maximum number of atoms allowed in this case is 1400 [4,5]. We employed an iterative solution scheme of the system of equations of this model as in Refs. [18,23]. In the case of ^{7}Li the attractive interaction is very weak and the the system of equations leads to rapid convergence. The condensate was described by the converged numerical solution of the Gross-Pitaevskii equation [14–17]. As the interaction is weak, the results for condensate fraction, chemical potential, and energy of ^{7}Li are very close to the corresponding results for the trapped ideal Bose gas. However, the deviation from the result of the ideal Bose gas in case of ^{7}Li is in the opposite direction compared to the corresponding deviation in case of repulsive interaction [18,23]. For example, in all cases the chemical potential is zero at the critical temperature. For ideal Bose gas it continues to be zero below the critical temperature. Below the critical temperature the chemical potential turns negative in case of ^{7}Li, whereas it turns positive in case of ^{87}Rb [23] where the interaction is repulsive. Although, in the present attractive case the number of particles in the condensate is small, the present results for the thermodynamic observables are quite reasonable physically. This demonstates that the mean-field two-fluid models [18,19,22,23] used to study the thermodynamic observables for the BE condensate in the repulsive case are quite useful in the attractive case also.

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